

Electronic and spin properties of Rashba billiards

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Ballistic electrons confined to a billiard and subject to spin-orbit coupling of the Rashba type are investigated, using both approximate semiclassical and exact quantum-mechanical methods. We focus on the low-energy part of the spectrum that has negative eigenvalues. When the spin precession length is smaller than the radius of the billiard, the low-lying energy eigenvalues turn out to be well described semiclassically. Corresponding eigenspinors are found to have a finite spin polarization in the direction perpendicular to the billiard plane.

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Spin-dependent phenomena in semiconductor nanostructures have become the focus of strong interest recently [1, 2]. In nonmagnetic systems, intriguing effects can arise from the presence of spin-orbit coupling. Structural inversion asymmetry in semiconductor heterostructures has been shown [3] to give rise to a spin splitting of the same type as was discussed in an early paper by Rashba [4]. Its tunability by external gate voltages [5, 6] has motivated the theoretical design of a spin-controlled field-effect transistor[7]. Novel spin properties arise from the interplay between Rashba spin splitting and further confinement of two-dimensional electrons in quantum wires [8, 9, 10, 11] or dots [12, 13, 14, 15, 16, 17]. Spin-orbit coupling has also been shown to affect the statistics of energy levels and eigenfunctions as well as current distributions [18, 19].

In this work, we study a *Rashba billiard*, i.e., non-interacting ballistic electrons moving in finite 2D regions whose dynamics is affected by the Rashba spin-orbit coupling. The Rashba spin-orbit coupling strength can be conveniently measured in terms of a wave-number scale $2k_{\text{so}}$, which corresponds to the Fermi-wave-vector difference for the two spin-split subbands. Typical values for the spin-orbit-induced spin precession length $L_{\text{so}} = \pi/k_{\text{so}}$ are of the order of a few hundred nanometers [1]. The relevant parameter characterizing a Rashba billiard of size L is $k_{\text{so}}L$. Taking $L = 10\mu\text{m}$ for a typical size of quantum dots, the relevant parameter in Rashba billiards can be as large as 70. Furthermore, the tunability of the Rashba spin-orbit coupling strength is a convenient tool to induced changes of the billiard's energy spectrum without applying external magnetic fields.

Below we present interesting features of the energy spectrum for Rashba billiards, focusing especially on its negative energy eigenvalues. We will show that the density of states (DOS) is singular at the bottom of the spectrum. This singular behavior occurs independently of the billiard's shape and is most striking if the Rashba parameter is large. We have found that for a circular shape, the

DOS has additional singularities at negative energies. We obtain analytic results for their positions. Their corresponding eigenspinors have a finite spin projection in the direction perpendicular to the billiard plane, which is the direct result of imposing hard-wall boundary conditions.

Our central quantity of interest is the Green's function for Rashba billiards. Having obtained it, we can derive the density of states (DOS) $\varrho(E)$ and the smooth counting function $\bar{N}(E)$, i.e., the leading Weyl law [20, 21], plus correction terms to it. (A discussion of these concepts for billiards without spin-orbit coupling can be found in Refs. 22, 23, 24, 25, 26.) We provide analytic results for circular Rashba billiards and give the first two leading terms for arbitrary shapes based on the image method of Berry and Mondragon [27]. The latter was developed for neutrino billiards, which have two-component wave functions and are rather similar to the Rashba billiards discussed here. Comparison of our analytical results from the semiclassical treatment to the numerically calculated exact energy levels of circular Rashba billiards demonstrate perfect agreement between the two. An asymptotic expansion of spinor wave functions for negative-energy eigenstates yields a finite spin polarization in the direction perpendicular to the billiard, in contrast to the familiar result for a 2D plane.

In the one-band effective-mass approximation the Hamiltonian with Rashba splitting in 2D is given by [28]

$$\hat{H} = \frac{p_x^2 + p_y^2}{2m^*} + \frac{\alpha}{\hbar} \hat{U} , \quad (1a)$$

$$\hat{U} = \sigma_x p_y - \sigma_y p_x , \quad (1b)$$

where σ_x, σ_y are Pauli matrices. This Hamiltonian governs the electron dynamics inside the billiard with Dirichlet boundary conditions at the perimeter. (See Ref. [29].) π/k_{so} is the spin-precession length, which can be tuned independently of the system size [5, 6, 7]. In the absence of any lateral confinement, the energy dispersion splits

into two branches [28]:

$$E(k_x, k_y) = \frac{\hbar^2}{2m^*} \left[(k \pm k_{\text{so}})^2 - k_{\text{so}}^2 \right], \quad (2)$$

where $k = \sqrt{k_x^2 + k_y^2}$. In the range $0 < k < k_{\text{so}}$, one branch has negative energies bounded from below by $-\Delta_{\text{so}} \equiv -\hbar^2 k_{\text{so}}^2 / (2m^*)$. The spin splitting is a consequence of broken spin-rotational invariance. The spin of energy eigenstates, which are labeled by a 2D vector \mathbf{k} , is polarized perpendicularly to \mathbf{k} [28]. Hence, no common spin quantization axis for single-electron states can be defined in the presence of spin-orbit coupling. At a given energy E , two propagating modes exist whose wave vectors can be found from the dispersion relation (2): $k_{\pm} = k \mp k_{\text{so}}$, where $k = \sqrt{\frac{2m^* E}{\hbar^2} + k_{\text{so}}^2}$.

The Hamiltonian \hat{H} commutes with the total angular momentum operator $\hat{J}_z = -i\hbar\partial_\varphi + \frac{\hbar}{2}\sigma_z$, where φ is the polar angle. The eigenspinors $|\chi_m^{(\pm)}\rangle$ corresponding to the two bands of the Hamiltonian (1) are given, in the representation of polar coordinates r, φ , by

$$\langle \mathbf{r} | \chi_m^{(\pm)} \rangle = \begin{pmatrix} \pm J_m(k_{\pm} r) \\ J_{m+1}(k_{\pm} r) e^{im\varphi} \end{pmatrix} e^{im\varphi}. \quad (3)$$

Here $J_m(x)$ is the Bessel function of integral order m and $E > -\Delta_{\text{so}}$. Other independent solutions can be obtained when $J_m(x)$ are replaced by $Y_m(x)$, $H_m^{(1)}(x)$, or $H_m^{(2)}(x)$. For Rashba billiards with arbitrary shape, the eigenstates can be expanded in the basis (3) using linear combinations of both \pm spinor states.

To proceed further, we need the free-space Green's function for the Rashba Hamiltonian (1). Using the fact that $\hat{U}^2 = p_x^2 + p_y^2$ the operator $\hat{G}_\infty = (E - \hat{H})^{-1}$ reads

$$\hat{G}_\infty = \frac{m^*}{\hbar^2} \frac{1}{k} \left[\left(k_+ + \hat{U} \right) \left(k_+^2 - \frac{\mathbf{p}^2}{\hbar^2} \right)^{-1} + \left(k_- - \hat{U} \right) \left(k_-^2 - \frac{\mathbf{p}^2}{\hbar^2} \right)^{-1} \right]. \quad (4)$$

Here E can be a complex number. We note that, for negative energies, the retarded Green's function contains incoming circular waves besides outgoing waves.

To satisfy the boundary conditions that $G(\mathbf{r}, \mathbf{r}')$ vanishes at the boundary, the Green's function is decomposed into two parts: $\hat{G} = \hat{G}_\infty + \hat{G}_H$, where the homogeneous part \hat{G}_H fulfills $(E - \hat{H}) \hat{G}_H = 0$. This latter Green's function is constructed, in the usual way, from the eigenspinors (3) as follows

$$\hat{G}_H = \sum_{m=-\infty}^{\infty} \left[A_m | \chi_m^{(+)} \rangle \langle \chi_m^{(+)} | + B_m | \chi_m^{(-)} \rangle \langle \chi_m^{(+)} | + C_m | \chi_m^{(+)} \rangle \langle \chi_m^{(-)} | + D_m | \chi_m^{(-)} \rangle \langle \chi_m^{(-)} | \right]. \quad (5)$$

The coefficients A_m, B_m, C_m and D_m should be chosen such that the total Green's function satisfies Dirichlet boundary conditions. In general, one gets an infinite set of inhomogeneous linear equations for the coefficients, which can be solved only numerically. The circular billiard is a special case for which the coefficients can be given analytically (not presented here) for any m .

From \hat{G} , the DOS can be obtained by $\varrho(E) = -\frac{1}{\pi} \lim_{\eta \rightarrow 0^+} \text{ImTr } \hat{G}(E + i\eta)$, where the trace means the limit $\mathbf{r} \rightarrow \mathbf{r}'$, integration of \mathbf{r} over the area of the billiard, and the trace in spin space. The counting function is defined by $N(E) = \int_{-\infty}^E \varrho(E') dE'$ and its smooth part $\bar{N}(E)$ requires averaging over a small energy range around E .

We now consider the circular Rashba billiard of radius R . Following the ideas of the systematic method of Berry and Howls [25], we have calculated the first few leading terms of $\bar{N}(E)$. (Details of the lengthy calculation will be published elsewhere.) The result is:

$$\bar{N}(\varepsilon) = \begin{cases} \frac{\varepsilon + 2\varepsilon_{\text{so}}}{2} - \sqrt{\varepsilon + \varepsilon_{\text{so}}} + \frac{2}{\pi} \left[\frac{\varepsilon}{\sqrt{\varepsilon + \varepsilon_{\text{so}}}} K \left(\sqrt{\frac{\varepsilon_{\text{so}}}{\varepsilon + \varepsilon_{\text{so}}}} \right) - \sqrt{\varepsilon + \varepsilon_{\text{so}}} E \left(\sqrt{\frac{\varepsilon_{\text{so}}}{\varepsilon + \varepsilon_{\text{so}}}} \right) \right], & \text{for } \varepsilon > 0, \\ \sqrt{\varepsilon_{\text{so}}} \sqrt{\varepsilon + \varepsilon_{\text{so}}} - \sqrt{\varepsilon + \varepsilon_{\text{so}}} - \frac{2\sqrt{\varepsilon_{\text{so}}}}{\pi} E \left(\sqrt{\frac{\varepsilon + \varepsilon_{\text{so}}}{\varepsilon_{\text{so}}}} \right), & \text{for } -\varepsilon_{\text{so}} < \varepsilon < 0, \end{cases} \quad (6)$$

where the dimensionless energies $\varepsilon = 2m^* E R^2 / \hbar^2$ and $\varepsilon_{\text{so}} = 2m^* \Delta_{\text{so}} R^2 / \hbar^2 = k_{\text{so}}^2 R^2$ have been introduced. Here $K(x)$ and $E(x)$ are the complete elliptic integrals of the first and second kind, respectively, with the same definitions as in Ref. 30. The first term for both positive and

negative energies is the contribution from \hat{G}_∞ , while the remainder originates from \hat{G}_H . We note that in a completely different context, namely for annular ray-splitting billiards, a similar Weyl formula has been calculated[31] involving also elliptic integrals.

For arbitrary shapes of Rashba billiards, we can also determine the area and the perimeter terms of the smooth part of the counting function. The largest contribution to $\bar{N}(E)$ comes from $\text{Tr } \hat{G}_\infty$, which is always proportional to the area A of the billiard:

$$\bar{N}_1(E) = \frac{Am^*}{2\pi\hbar^2} \begin{cases} \frac{E}{2} + \Delta_{\text{so}}, & \text{for } E > 0, \\ \sqrt{\Delta_{\text{so}}}\sqrt{E + \Delta_{\text{so}}}, & \text{for } -\Delta_{\text{so}} < E < 0. \end{cases} \quad (7)$$

It follows directly from Eq. (7) that, for negative energies, the DOS shows a $1/\sqrt{E + \Delta_{\text{so}}}$ singularity at the bottom of the spectrum $E \rightarrow -\Delta_{\text{so}}$. The perimeter term can be derived from the generalization of the image method of Ref. 23 using only the free space Green's function. The calculation is very much similar to that applied by Berry and Mondragon [27] for neutrino billiards and yields

$$\bar{N}_2(E) = -\frac{\mathcal{L}}{2\pi} \sqrt{\frac{2m^*}{\hbar^2}} \sqrt{E + \Delta_{\text{so}}}, \quad (8)$$

valid for all energies $E > -\Delta_{\text{so}}$. Here \mathcal{L} is the perimeter length of the billiard. The minus sign is a consequence of Dirichlet boundary conditions. For zero spin-orbit coupling, $\bar{N}_1(E) + \bar{N}_2(E)$ coincides with the previously derived result for 2D billiards [21] (apart from a factor 2 due to spin). The area term (7) can alternatively be derived from the classical phase-space integral in the underlying classical approach. However, the classical dynamics of electrons in Rashba billiards is described by *two* Hamiltonians [32], which are reminiscent of the two dispersion branches (2). The constant-energy surfaces in phase space are different for the two Hamiltonians, yielding different contributions to the classical phase-space integral. A simple calculation gives then Eq. (7).

To get better agreement between the numerically obtained exact counting function and $\bar{N}(E)$ one should calculate further terms besides $\bar{N}_1(E)$ and $\bar{N}_2(E)$ for large k_{so} . This motivated us to consider more corrections in Eq. (6) involving elliptic integrals. For the case of circular Rashba billiards, the Schrödinger equation is separable in polar coordinates. The resulting radial equation for both spinor components leads to the secular equation [33] $J_m(k_+R)J_{m+1}(k_-R) + J_m(k_-R)J_{m+1}(k_+R) = 0$, where m is an integer. This equation is invariant under the change $m \rightarrow -m-1$ (Kramers degeneracy). Formal solutions of the secular equation having zero wave vector are excluded since the corresponding wave functions vanish everywhere inside the billiard. We obtain the exact $N(\varepsilon)$ from our solutions of the secular equation for different m . In Fig. 1a, we plot the difference $\Delta N = N(\varepsilon) - \bar{N}(\varepsilon)$ as a function of the dimensionless energy ε . The difference fluctuates around zero, which shows we did not miss levels (the mean value of ΔN is a sensitive test for missing levels, see e.g., Ref. 34). Fig. 1a shows data for approximately 54570 levels. Without correction terms in Eq. (6) with elliptic integrals, ΔN would increase monotonically

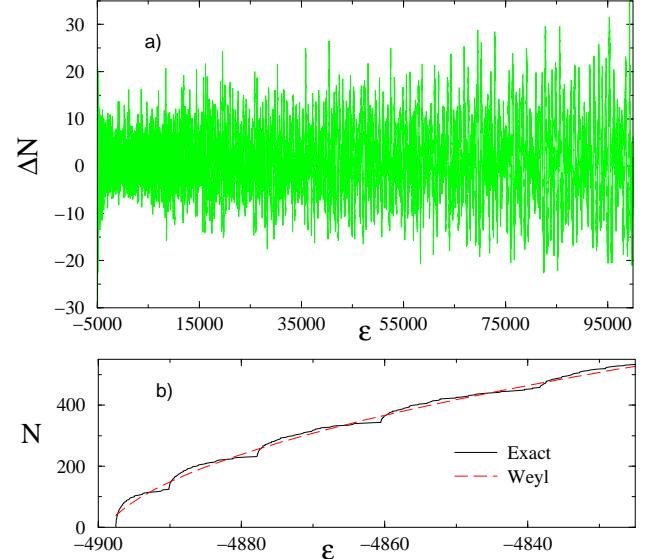


FIG. 1: In panel a) the difference ΔN between the exact counting function and $\bar{N}(\varepsilon)$ from Eq. (6) is plotted for $\sqrt{\varepsilon_{\text{so}}} = k_{\text{so}}R = 70$. In panel b) the exact counting function (solid line) and $\bar{N}(\varepsilon)$ (dashed line) are shown. In both panels dimensionless energies $\varepsilon = 2m^*ER^2/\hbar^2$ are used.

on average, and would predict ≈ 70 missing levels in the energy range plotted.

In Fig. 1b, the exact counting function is shown together with the Weyl formula (6) for negative energies near the bottom of the spectrum $-\varepsilon_{\text{so}}$. The overall agreement is good but the exact $N(\varepsilon)$ shows an additional rounded step structure at certain energies ε_n . This feature shows up only for negative energies, although for larger energies this is less pronounced. The step structure results in large deviations ΔN at energies ε_n and concomitant large peaks in the DOS. To see the reason for this behavior, it is useful to plot the energy levels as functions of m , as shown in Fig. 2. The curves in the figure start almost horizontally at ε_n , $n = 1, 2, \dots$ resulting in large peaks in the DOS at the same energies.

Using Hankel's asymptotic expression for Bessel functions with large argument [35], we were able to derive the energy dispersion accurately in next-to-leading order:

$$\varepsilon_{m,n} = \left(\frac{n\pi}{2}\right)^2 - \varepsilon_{\text{so}} + \delta_{m,n} \quad , \quad (9a)$$

$$\delta_{m,n} = \left(\frac{n\pi}{2}\right)^2 \frac{2m+1}{\varepsilon_{\text{so}}} [m+1 + (-1)^n \cos(2\sqrt{\varepsilon_{\text{so}}})] \quad (9b)$$

valid only for negative energies and $n = 1, 2, \dots, \text{int}(2\sqrt{\varepsilon_{\text{so}}}/\pi)$. For small m, n the above expression agrees excellently with the numerics (e.g., $\varepsilon_{0,1}$ is accurate up to 8 digits for $\varepsilon_{\text{so}} = 70$). It is straightforward to obtain corresponding spinor eigenstates and calculate their expectation value for the z component of spin. Similar to the case of Rashba-split

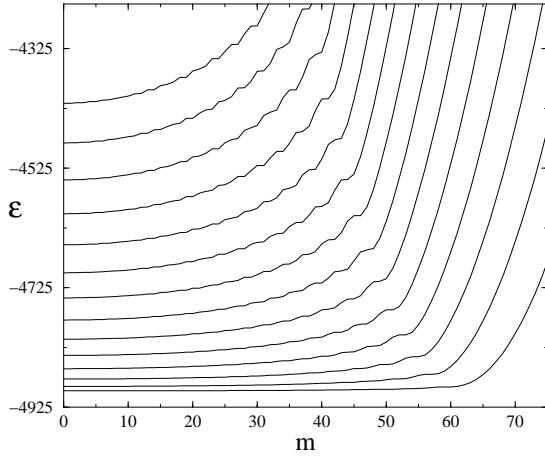


FIG. 2: The energy levels (in units of $2m^*R^2/\hbar^2$) of circular Rashba billiards as functions of m . For a given m levels are ordered and first, second, etc. energies are connected as m varies.

eigenstates in rings [36], but in contrast to that of quantum wires [8, 10], it turns out to be finite. We find

$$\langle \sigma_z \rangle_{m,n} = -\frac{\left(\frac{n\pi}{2\sqrt{\varepsilon_{\text{so}}}}\right)^2 \cos(2\sqrt{\varepsilon_{\text{so}}})}{(2m+1)\cos(2\sqrt{\varepsilon_{\text{so}}}) + 2(-1)^{n+m}\frac{\varepsilon_{\text{so}} - (\frac{n\pi}{2})^2}{\sqrt{\varepsilon_{\text{so}}}}} \quad (10)$$

The Schrödinger equation (including boundary conditions) for circular Rashba billiards is separable in polar coordinates, thus integrable. Hence, all the level statistics should be Poissonian (see e.g. Ref. 37). Indeed, we have found that the nearest-neighbor level-spacing distribution $P(s)$ is Poissonian (not shown here). For other shapes, the spin-orbit coupling destroys the integrability. Random Matrix Theory predicts the statistics to be that of the Gaussian Orthogonal Ensemble (GOE) due to time reversal symmetry [9]. Some other intermediate distribution [19] has been found for rectangular shape and for small k_{so} , reflecting the fact that the rectangular billiard without SO coupling is integrable.

Finally, a few interesting open theoretical problems are listed. The Weyl formula is essential to develop a periodic orbit theory for Rashba billiards. (For normal billiards, see Brack and Bhaduri's book in Ref. 21, and a theory in case of harmonically confined Rashba systems is given in Ref. 32.) The Green's function method presented in this work would be a suitable starting point to calculate observables such as the magnetization [38] or persistent currents [36] in Rashba billiards.

In conclusion, we have presented a study of electron billiards with spin-dependent dynamics due to Rashba spin splitting. Semiclassical results for the spectrum agree well with exact quantum calculations. We find interesting properties of negative-energy states, including a finite spin projection in the out-of-plane direction.

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